

```
ring nodes:
    1 2 3 4 5 6 7 8 9 10

chain bonds:
    7-13 16-17

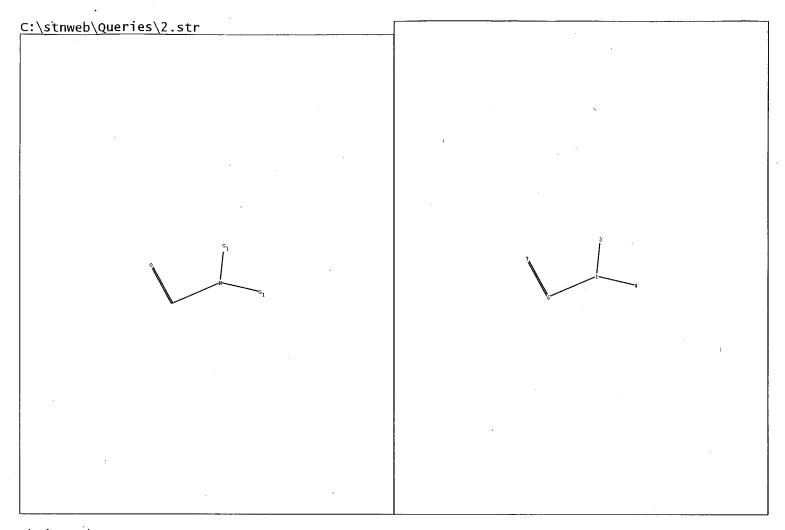
ring bonds:
    1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10

exact/norm bonds:
    7-13 16-17

normalized bonds:
    1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10

isolated ring systems:
    containing 1:
```

Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS



chain nodes:
 1 3 4 6 7
chain bonds:
 1-4 1-3 1-6 6-7
exact/norm bonds:
 1-4 1-3 1-6 6-7

G1:CH3,Et

Match level: 1:CLASS 3:CLASS 4:CLASS 6:CLASS 7:CLASS `

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```
1 2 3
                             10
                                29
                                     30
                                        31
                                            32
                                                33
chain bonds :
   7-13 16-17 20-21 20-25
                            20-24 21-22
                                          31-35
                                                38-39
                                                        38-40 42-43
ring bonds :
   1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10
                                          7-8 8-9 9-10 29-30 29-34 30-31 31-32
   32-33 33-34
exact/norm bonds :
   7-13 16-17 20-21 20-25 20-24 21-22
                                         38-39 38-40 42-43
exact bonds :
   31-35
normalized bonds :
   1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 29-30 29-34 30-31 31-32
   32-33. 33-34
isolated ring systems :
   containing 1 : 29 :
G1:CH3,Et
Match level:
   1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:CLASS
   12:CLASS 13:CLASS 14:CLASS
                               15:CLASS 16:CLASS 17:CLASS 18:CLASS 20:CLASS 21:CLASS
   22:CLASS
             24:CLASS
                      25:CLASS
                               29:Atom 30:Atom 31:Atom 32:Atom 33:Atom 34:Atom
   35:CLASS
             36:CLASS
                     37:CLASS 38:CLASS 39:CLASS 40:CLASS 41:CLASS 42:CLASS 43:CLASS
   44:CLASS
fragments assigned reactant role:
   containing 29
fragments assigned product role:
   containing 1
fragments assigned reactant/reagent role:
```

35

36

38

39

40 42 43

chain nodes :

ring nodes :

11 13 14 16 17

containing 20

20

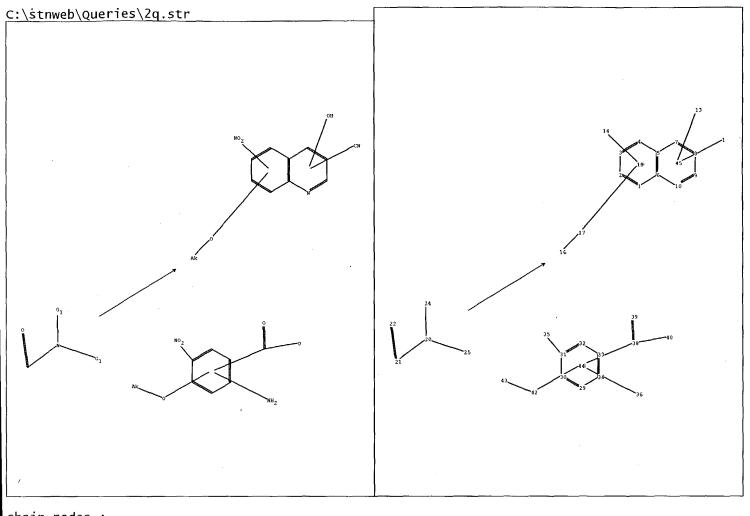
21

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```
chain nodes :
   11 13 14 16 17 20
                                   24
                                        25
                                            35
                                                36
                                                    38
                                                        39
                                                            40 42 43
                           21 22
ring nodes :
    1 2 3 4 5 6 7
                               10
                                  29
                                       30
                                           31
                                               32
chain bonds :
    16-17 20-21 20-25 20-24 21-22
                                       31-35 38-39 38-40 42-43
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 29-30 29-34 30-31 31-32 32-33 33-34 exact/norm bonds:
    16-17 20-21 20-25 20-24 21-22 38-39 38-40 42-43
exact bonds :
    31-35
normalized bonds :
    1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 29-30 29-34 30-31 31-32
    32-33 33-34
isolated ring systems : containing 1 : 29 :
```

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 20:CLASS 21:CLASS 22:CLASS 24:CLASS 25:CLASS 29:Atom 30:Atom 31:Atom 32:Atom 33:Atom 34:Atom 35:CLASS 36:CLASS 37:CLASS 38:CLASS 39:CLASS 40:CLASS 41:CLASS 42:CLASS 43:CLASS

G1:CH3,Et

Match level :

44:CLASS 45:CLASS

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SINCE FILE TOTAL ENTRY SESSION 0.21 0.21

FULL ESTIMATED COST

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STRUCTURE FILE UPDATES: 25 OCT 2004 HIGHEST RN 769101-30-6 DICTIONARY FILE UPDATES: 25 OCT 2004 HIGHEST RN 769101-30-6

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

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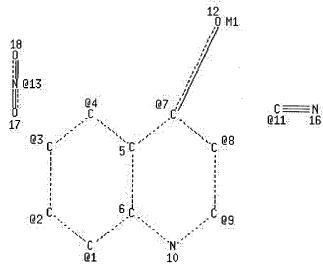
=>

L1STRUCTURE UPLOADED

=> d 11

L1 HAS NO ANSWERS

STR



Page 1-A



Page 2-A

VPA 11-7/8/9 S

VPA 13-2/3/4 s

VPA 15-1/2/3 S

| NODE AT | 'TRII | BUTES: | | |
|---------|-------|--------|------------------------|----|
| HCOUNT | IS | M1 | AT | 12 |
| NSPEC | IS | R | AT | 1 |
| NSPEC | IS | R | AT | 2 |
| NSPEC | IS | R | AT | 3 |
| NSPEC | IS | R | AT | 4 |
| NSPEC | IS | R | $\mathbf{T}\mathbf{A}$ | 5 |
| NSPEC | IS | R | AT | 6 |
| NSPEC | IS | R | AT | 7 |
| NSPEC | IS | R | AT | 8 |
| NSPEC | IS | R | AT | 9 |
| NSPEC | IS | R | AT | 10 |
| NSPEC | TS | C | ידי מ | 11 |

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IS C
NSPEC
                  AT
                     12
      IS C
NSPEC
                  AT
                      13
       IS C
NSPEC
                  AT
                      14
      IS C
NSPEC
                  AT
                      15
      IS C
NSPEC
                  AT 16
NSPEC
      IS C
                  AT
                      17
NSPEC
       IS C
                  AT 18
DEFAULT MLEVEL IS ATOM
MLEVEL IS CLASS AT 11 12 13 14 15 16 17 18
DEFAULT ECLEVEL IS LIMITED
GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS 18
STEREO ATTRIBUTES: NONE
=> s 11
SAMPLE SEARCH INITIATED 01:40:55 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -
                                     16 TO ITERATE
100.0% PROCESSED
                 16 ITERATIONS
                                                               1 ANSWERS
SEARCH TIME: 00.00.01
FULL FILE PROJECTIONS: ONLINE **COMPLETE**
                        BATCH
                                **COMPLETE**
PROJECTED ITERATIONS:
                                80 TO
                                           560
PROJECTED ANSWERS:
                                1 TO
                                           8.0
L2
              1 SEA SSS SAM L1
=> s li full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:Y
FULL SEARCH INITIATED 01:40:59 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 189 TO ITERATE
100.0% PROCESSED
                     189 ITERATIONS
                                                               5 ANSWERS
SEARCH TIME: 00.00.01
L3
              5 SEA SSS FUL L1
=>
L4
       STRUCTURE UPLOADED
=> 3 14
L4 HAS NO ANSWERS
               STR
=> 5 14
SAMPLE SEARCH INITIATED 01:43:05 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 268233 TO ITERATE
  0.4% PROCESSED
                   1000 ITERATIONS
                                                              18 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01
```

ONLINE **INCOMPLETE**

INCOMPLETE

BATCH

FULL FILE PROJECTIONS:

```
PROJECTED ITERATIONS:
                           EXCEEDS 1000000
PROJECTED ANSWERS:
                           EXCEEDS
L5
             18 SEA SSS SAM L4
=> e dimethyl formamide/cn
E.1
             1
                   DIMETHYL FLUOROPHOSPHATE/CN
F.2
                   DIMETHYL FORMAL/CN
Е3
             0 --> DIMETHYL FORMAMIDE/CN
                   DIMETHYL FORMAMIDOMALONATE/CN
E.4
             1
E5
             1
                   DIMETHYL FORMYLMALONATE/CN
F.6
             1
                   DIMETHYL FORMYLPHOSPHONATE/CN
E7
             1
                   DIMETHYL FORMYLSUCCINATE/CN
Ε8
                   DIMETHYL FUMARATE/CN
                   DIMETHYL FUMARATE HOMOPOLYMER/CN
Ε9
             1
E10
             1
                   DIMETHYL FUMARATE POLYMER/CN
E11
             1
                   DIMETHYL FUMARATE RADICAL ION(1-)/CN
E12
             1
                   DIMETHYL FUMARATE-1,1'-(1,2-ETHANEDIYL)BIS(2,2,6,6-TETRAMETH
                   YL-4-PIPERIDINOL) COPOLYMER/CN
=> e dimethyl formamide/cn
E1
             1
                   DIMETHYL FLUOROPHOSPHATE/CN
E2
                   DIMETHYL FORMAL/CN
             1
E3
             0 --> DIMETHYL FORMAMIDE/CN
E4
             1
                   DIMETHYL FORMAMIDOMALONATE/CN
E5
             1
                   DIMETHYL FORMYLMALONATE/CN
E6
             1
                   DIMETHYL FORMYLPHOSPHONATE/CN
E7
                   DIMETHYL FORMYLSUCCINATE/CN
E.8
             1
                   DIMETHYL FUMARATE/CN
Ε9
             1
                   DIMETHYL FUMARATE HOMOPOLYMER/CN
E10 -
             1
                   DIMETHYL FUMARATE POLYMER/CN
E11
             1
                   DIMETHYL FUMARATE RADICAL ION(1-)/CN
E12
                   DIMETHYL FUMARATE-1,1'-(1,2-ETHANEDIYL)BIS(2,2,6,6-TETRAMETH
                   YL-4-PIPERIDINOL) COPOLYMER/CN
=> e t-butyl cyanoacetate/cn
E1
             1
                   T-BUTYL 6-TRIFLUOROMETHYL-3-(4-PYRIDINYLAMINO)INDOLE-2-CARBO
                   XYLATE/CN
E2
                   T-BUTYL ACRYLATE-DIETHYLENE GLYCOL MONOETHYL ETHER ACRYLATE-
                   BUTYL METHACRYLATE-METHYL METHACRYLATE-METHACRYLIC ACID-DI-T
                   -BUTYL MALEATE COPOLYMER/CN
E3
             0 --> T-BUTYL CYANOACETATE/CN
E4
                   T-BUTYL ETHYL KETONE/CN
E5
             1
                   T-BUTYL HYDROPEROXIDE/CN
E6
             1
                   T-BUTYL IODIDE/CN
E7
             1
                   T-BUTYL METHACRYLATE-1, 3-BUTYLENE GLYCOL DIMETHACRYLATE COPO
                   LYMER/CN
E8
             1
                   T-BUTYL METHACRYLATE-DIETHYLENE GLYCOL MONOETHYL ETHER ACRYL
                   ATE-2-HYDROXYETHYL METHACRYLATE COPOLYMER/CN
E9
                   T-BUTYL METHACRYLATE-DIETHYLENE GLYCOL MONOETHYL ETHER ACRYL
                   ATE-METHACRYLIC ACID COPOLYMER/CN
E10
             1
                   T-BUTYL METHACRYLATE-DIPROPYLENE GLYCOL MONOMETHYL ETHER ACR
                   YLATE-METHACRYLIC ACID COPOLYMER/CN
E11
                   T-BUTYL METHACRYLATE-ETHYLENE GLYCOL MONOPHENYL ETHER METHAC
                   RYLATE-METHACRYLIC ACID COPOLYMER/CN
E12
             1
                   T-BUTYL METHACRYLATE-ETHYLENE GLYCOL MONOPHENYL ETHER METHAC
                   RYLATE-METHACRYLIC ACID-METHYL METHACRYLATE COPOLYMER/CN
```

=> d his

(FILE 'HOME' ENTERED AT 01:37:40 ON 27 OCT 2004)

FILE 'REGISTRY' ENTERED AT 01:37:49 ON 27 OCT 2004

L1 STRUCTURE UPLOADED

L2 1 S L1

L3 5 S L1 FULL

L4 STRUCTURE UPLOADED

L5 18 S L4

E DIMETHYL FORMAMIDE/CN

E DIMETHYL FORMAMIDE/CN

E T-BUTYL CYANOACETATE/CN

=> file hcaplus

COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION

159.83

159.62

FULL ESTIMATED COST

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FILE 'REGISTRY' ENTERED AT 01:37:49 ON 27 OCT 2004
L1 STRUCTURE UPLOADED
L2 1 S L1
L3 5 S L1 FULL
L4 STRUCTURE UPLOADED

E DIMETHYL FORMAMIDE/CN
E DIMETHYL FORMAMIDE/CN
E T-BUTYL CYANOACETATE/CN

FILE 'HCAPLUS' ENTERED AT 01:44:10 ON 27 OCT 2004

=> s 13 L6 11 L3

=> s 13/prep

h

L5

18 S L4

11 L3 3214460 PREP/RL 11 L3/PREP (L3 (L) PREP/RL)

=> file reg

L7

COST IN U.S. DOLLARS

SINCE FILE TOTAL

ENTRY SESSION

FULL ESTIMATED COST

2.36 162.19

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|------|----|--|--|--|--|
| E1 | 1 | DIMETHYLFLUOROSILYL (TRICHLOROGERMYL) METHANE/CN | | | |
| E2 - | 1 | DIMETHYLFORMALDEHYDE/CN | | | |
| ,E3 | 1> | DIMETHYLFORMAMIDE/CN | | | |
| | 1 | DIMETHYLFORMAMIDE 2,4-DINITROPHENYLHYDRAZONE/CN | | | |
| E5 | 1 | DIMETHYLFORMAMIDE AZINE/CN | | | |
| | 1 | DIMETHYLFORMAMIDE COMPLEX WITH MOL. IODINE (1:1)/CN | | | |
| E7 | 1 | DIMETHYLFORMAMIDE COMPOUND WITH CARBON TETRACHLORIDE (1:1)/C | | | |
| | | N | | | |
| E8 | 1 | DIMETHYLFORMAMIDE COMPOUND WITH SULFUR TRIOXIDE (1:1)/CN | | | |
| E9 | 1 | DIMETHYLFORMAMIDE COMPOUND WITH WATER (1:1)/CN | | | |
| | 1 | DIMETHYLFORMAMIDE COMPOUND WITH WATER (2:1)/CN | | | |
| E11 | 1 | DIMETHYLFORMAMIDE CYCLIC ETHYLENE ACETAL/CN | | | |
| E12 | 1 | DIMETHYLFORMAMIDE DEMETHYLASE/CN | | | |
| | | | | | |

=> s e3

L8 1 DIMETHYLFORMAMIDE/CN

=> file hcaplus

COST IN U.S. DOLLARS

SINCE FILE TOTAL

FULL ESTIMATED COST

ENTRY SESSION 4.85 167.04

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=> s 18/rct

27195 L8

2670391 RCT/RL

L9 4103 L8/RCT

(L8 (L) RCT/RL)

=> d his

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L1 STRUCTURE UPLOADED

L2 1 S L1

L3 5 S L1 FULL

L4 STRUCTURE UPLOADED

L5 18 S L4

E DIMETHYL FORMAMIDE/CN

E DIMETHYL FORMAMIDE/CN

E T-BUTYL CYANOACETATE/CN

FILE 'HCAPLUS' ENTERED AT 01:44:10 ON 27 OCT 2004

L6 11 S L3

L7 11 S L3/PREP

FILE 'REGISTRY' ENTERED AT 01:44:36 ON 27 OCT 2004

E DIMETHYLFORMAMIDE/CN

L8 1 S E3

FILE 'HCAPLUS' ENTERED AT 01:44:50 ON 27 OCT 2004

L9 4103 S L8/RCT

=> s 19 and 17

L10 1 L9 AND L7

=> d 110, ibib abs hitstr, 1

L10 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2004 ACS on STN



ACCESSION NUMBER:

1999:794373 HCAPLUS

DOCUMENT NUMBER:

132:35620

TITLE:

Preparation of substituted 3-cyanoquinolines as

inhibitors of growth factor receptor protein tyrosine

kinases (PTK)

INVENTOR(S):

Wissner, Allan: Johnson, Bernard D.; Reich, Marvin F.;

Floyd, Middleton B), Jr.; Kitchen, Douglas B.; Tsou,

Hwei-ru

PATENT ASSIGNEE(S):

American Cyanamid Co., USA

SOURCE:

U.S., 80 pp. CODEN: USXXAM

DOCUMENT TYPE:

LANGUAGE:

Patent English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

| | PATENT NO. | KIND | DATE | APPLICATION NO. | | DATE |
|-----|---------------------|--------|-----------|-----------------|---|----------|
| | | | | | - | |
| | US 6002008 | A | 19991214 | US 1998-49718 | | 19980327 |
| PR1 | ORITY APPLN. INFO.: | | | US 1997-41963P | P | 19970403 |
| OTH | HER SOURCE(S): | MARPAT | 132:35620 | | | |
| GI | | | | | | |

This invention provides compds. having the formula (I; wherein: X is AΒ cycloalkyl which may be optionally substituted; or is a pyridinyl, pyrimidinyl, or Ph ring; wherein the pyridinyl, pyrimidinyl, or Ph ring may be optionally substituted; n is 0-1; Y is NH, O, S, or NR; R is alkyl of 1-6 carbon atoms; R1, R2, R3, and R4 are each, independently, hydrogen, halogen, alkyl, alkenyl, alkynyl, alkenyloxy, alkynoyloxy, hydroxymethyl, halomethyl, alkanoyloxy, alkenoyloxy, alkynyloxy, alkanoyloxymethyl, alkenoyloxymethyl, alkynoyloxymethyl, alkoxymethyl, alkoxy, alkylthio, alkylsulphinyl, alkylsulfonyl, alkylsulfonamido, alkenylsulfonamido, alkynylsulfonamido, hydroxy, trifluoromethyl, cyano, nitro, carboxy, carboalkoxy, carboalkyl, phenoxy, Ph, thiophenoxy, benzyl, amino, hydroxyamino, alkoxyamino, alkylamino, dialkylamino, aminoalkyl, N-alkylaminoalkyl, N,N-dialkylaminoalkyl, phenylamino, benzylamino, etc.; R5 is alkyl which may be optionally substituted, or Ph which may be optionally substituted; R6 is hydrogen, alkyl, or alkenyl; R7 is chloro or bromo; R8 is hydrogen, alkyl, aminoalkyl, N-alkylaminoalkyl, N, N-dialkylaminoalkyl, N-cycloalkylaminoalkyl, N-cycloalkyl-N-

ΙI

alkylaminoalkyl, N, N-dicycloalkylaminoalkyl, morpholino-N-alkyl, piperidino-N-alkyl, N-alkyl-piperidino-N-alkyl, azacycloalkyl-N-alkyl, hydroxyalkyl, alkoxyalkyl, carboxy, carboalkoxy, Ph, carboalkyl, chloro, fluoro, or bromo; Z is amino, hydroxy, alkoxy, alkylamino, dialkylamino). The compds. of the present invention inhibit the action of certain growth factor receptor protein tyrosine kinases (PTK) thereby inhibiting the abnormal growth of certain cell types. They are therefore useful for the treatment of certain diseases that are the result of deregulation of these PTKs, in particular as anti-cancer agents for the treatment of cancers expressing epidermal growth factor receptor (EGFR), mitogen activated protein kinase (MAPK), epithelial kinase (ECK), and kinase insert domain contg. receptor (KDR) in mammals and for the treatment of polycystic kidney disease in mammals. Thus, To a mixt. of 1.9 g (5.1 mmol) of 4-[(3-bromophenyl)amino]-7-methoxy-6-amino-3-quinolinecarbonitrile and 5.3 mL (31 mmol) of Hunig's base in 110 mL of dry THF at 0° C., with stirring, was added a THF soln. contg. 5.7 g (31 mmol) of 4-bromocrotonyl chloride dropwise. The mixt. was stirred for addnl. 0.5 h. After addn. 100 mL of satd. sodium chloride soln. was added to the reaction mixt., then it was extd. with Et acetate. The Et acetate soln. was dried over sodium sulfate and then was added to 40 mL of di-Me amine soln. (2.0 M in THF) at 0° dropwise and stirred an addnl. 0.5 h to give 4-Dimethylamino-but-2-enoic acid [4-(3-bromo-phenylamino)-3-cyano-7methoxy-quinolin-6-yl]amide (II). II showed IC50 of 0.000008 μM against epidermal growth factor receptor kinase.

IT <u>68-12-2</u>, DMF, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. of substituted 3-cyanoquinolines as inhibitors of growth factor receptor protein tyrosine kinases (PTK) for treatment of cancers and polycystic kidney disease)

RN 68-12-2 HCAPLUS

CN Formamide, N, N-dimethyl- (8CI, 9CI) (CA INDEX NAME)

IT 27333-44-4P 214476-08-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(prepn. of substituted 3-cyanoquinolines as inhibitors of growth factor receptor protein tyrosine kinases (PTK) for treatment of cancers and polycystic kidney disease)

RN 27333-44-4 HCAPLUS

CN 3-Quinolinecarbonitrile, 4-hydroxy-8-methoxy-6-nitro- (8CI, 9CI) (CA INDEX NAME)

h

RN 214476-08-1 HCAPLUS

CN 3-Quinolinecarbonitrile, 7-ethoxy-4-hydroxy-6-nitro- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d his

(FILE 'HOME' ENTERED AT 01:37:40 ON 27 OCT 2004)

29

FILE 'REGISTRY' ENTERED AT 01:37:49 ON 27 OCT 2004

L1 STRUCTURE UPLOADED

L2 1 S L1

L3 5 S L1 FULL

L4 STRUCTURE UPLOADED

L5 18 S L4

E DIMETHYL FORMAMIDE/CN

E DIMETHYL FORMAMIDE/CN

E T-BUTYL CYANOACETATE/CN

FILE 'HCAPLUS' ENTERED AT 01:44:10 ON 27 OCT 2004

L6 11 S L3

L7 11 S L3/PREP

FILE 'REGISTRY' ENTERED AT 01:44:36 ON 27 OCT 2004

E DIMETHYLFORMAMIDE/CN

L8 1 S E3

FILE 'HCAPLUS' ENTERED AT 01:44:50 ON 27 OCT 2004

L9 4103 S L8/RCT

L10 1 S L9 AND L7

=> file caold

COST IN U.S. DOLLARS SINCE FILE TOTAL

ENTRY SESSION

FULL ESTIMATED COST 7.12 174.16

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL

ENTRY SESSION

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FILE COVERS 1907-1966

FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

This file supports REG1stRY for direct browsing and searching of all substance data from the REGISTRY file. Enter $\underline{\text{HELP FIRST}}$ for more information.

=> d his

(FILE 'HOME' ENTERED AT 01:37:40 ON 27 OCT 2004)

FILE 'REGISTRY' ENTERED AT 01:37:49 ON 27 OCT 2004

L1 STRUCTURE UPLOADED

L2 1 S L1

L3 5 S L1 FULL

L4 STRUCTURE UPLOADED

L5 18 S L4

E DIMETHYL FORMAMIDE/CN

E DIMETHYL FORMAMIDE/CN

E T-BUTYL CYANOACETATE/CN

FILE 'HCAPLUS' ENTERED AT 01:44:10 ON 27 OCT 2004

L6 11 S L3

L7 11 S L3/PREP

FILE 'REGISTRY' ENTERED AT 01:44:36 ON 27 OCT 2004

E DIMETHYLFORMAMIDE/CN

L8 1 S E3

FILE 'HCAPLUS' ENTERED AT 01:44:50 ON 27 OCT 2004

L9 4103 S L8/RCT

L10 1 S L9 AND L7

FILE 'CAOLD' ENTERED AT 01:45:24 ON 27 OCT 2004

=> s 13 and 18

0 L3

17 L8

L11 0 L3 AND L8

=> file casreact

COST IN U.S. DOLLARS

SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST

0.42
174.58

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL
ENTRY SESSION

CA SUBSCRIBER PRICE ENTRY SESSION 0.00 -0.70

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FILE CONTENT: 1840 - 24 Oct 2004 VOL 141 ISS 17

CASREACT now has more than 8 million reactions

h

Some CASREACT records are derived from the ZIC/VINITI database (1974-1991) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> L12

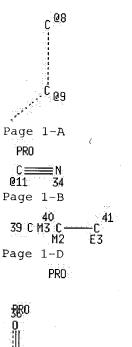
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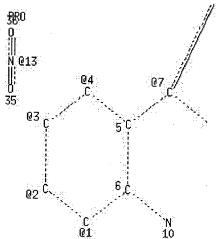
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L12 HAS NO ANSWERS

L12

12 0 M1





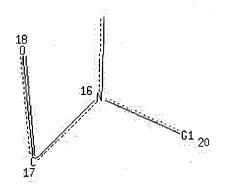
Page 1-F

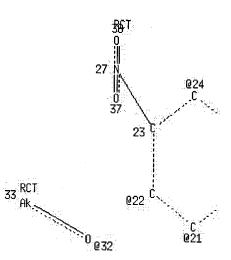


RRT 19

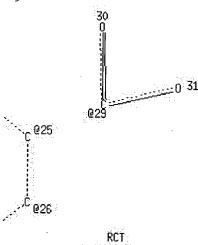
Page 2-E

RCT Page 2-F





Page 3-E



028 N M2

Page 3-F VAR G1=39/40

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VPA 13-2/3/4 S
VPA 15-1/2/3 S
VPA 28-21/25/26 S
VPA 29-24/25/26 S
VPA 32-21/22/24 S
NODE ATTRIBUTES:
HCOUNT
        IS M1
                    TA
                        12
         IS M2
                        28
HCOUNT
                    AT
HCOUNT
         IS M3
                    AT
                        39
HCOUNT
         IS M2
                        40
                    AT
HCOUNT
         IS E3
                    ΑT
                        41
NSPEC
         IS R
                    AT
                         1
NSPEC
         IS R
                    ΑT
NSPEC
         IS R
                    AT
                         3
NSPEC
         IS R
                    ΑT
                          4
NSPEC
                         5
         IS R
                    AT
NSPEC
         IS R
                    AT
                          6
NSPEC
         IS R
                    AT
                         7
NSPEC
         IS R
                    ΑT
                          8
NSPEC
                         9
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NSPEC
        IS R
                    AT
                        10
NSPEC
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                    AT
                        11
NSPEC
         IS C
                    ΑT
                        12
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         IS C
                        13
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NSPEC
         IS C
                    ΑT
                        14
NSPEC
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                    AT
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NSPEC
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                    ΑT
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NSPEC
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NSPEC
                    AT
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NSPEC
         IS C
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                        37
NSPEC
         IS C
                   AT
                        38
DEFAULT MLEVEL IS ATOM
                        11 12 13 14 15 16 17 18 27 28 29 30 31 32 33 34 35
        IS CLASS AT
           36 37 38 39 40 41
DEFAULT ECLEVEL IS LIMITED
GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS
```

 $h \qquad \qquad eb \ c \qquad g \ cg \ b \qquad cg$

STEREO ATTRIBUTES: NONE

```
=> s 112
```

SAMPLE SEARCH INITIATED 01:51:30 FILE 'CASREACT'

SCREENING COMPLETE - 0 REACTIONS TO VERIFY FROM 0 DOCUMENTS

100.0% DONE 0 VERIFIED 0 HIT RXNS

0 DOCS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED VERIFICATIONS: PROJECTED ANSWERS:

0 TO 0 0 TO

0 SEA SSS SAM L12 (0 REACTIONS)

=> s 112 full

THE ESTIMATED SEARCH COST FOR FILE 'CASREACT' IS 102.30 U.S. DOLLARS DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:v FULL SEARCH INITIATED 01:51:36 FILE 'CASREACT'

SCREENING COMPLETE - 4 REACTIONS TO VERIFY FROM 1 DOCUMENTS

100.0% DONE 4 VERIFIED 0 HIT RXNS

0 DOCS

SEARCH TIME: 00.00.01

L14

L13

0 SEA SSS FUL L12 (0 REACTIONS)

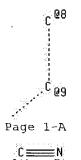
L15 STRUCTURE UPLOADED

=> d 115

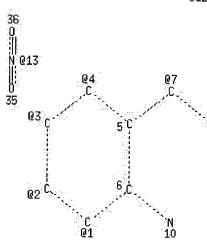
L15 HAS NO ANSWERS

L15 STR

0 M1

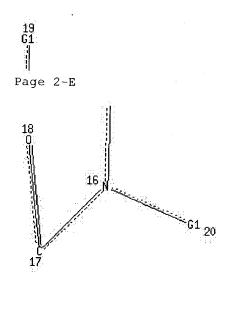


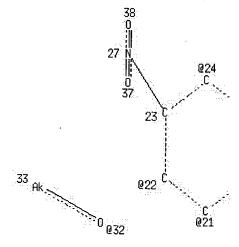
Page 1-D



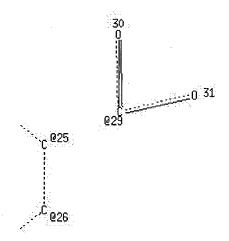
Page 1-F







Page 3-E



Q28 N M2

Page 3-F

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VAR G1=39/40
VPA 11-7/8/9 S
VPA 13-2/3/4 S
VPA 15-1/2/3 S
VPA 28-21/25/26 S
VPA 29-24/25/26 S
VPA 32-21/22/24 S
VPA 12-7/8 S
NODE ATTRIBUTES:
HCOUNT
         IS M1
                    AT
                         12
HCOUNT
         IS M2
                         28
                    TA
HCOUNT
         IS M3
                    AT
                         39
HCOUNT
         IS M2
                         40
                    AT
HCOUNT
         IS E3
                         41
                    AT
NSPEC
         IS R
                    AT
                          1
NSPEC
         IS R
                    AT
                          2
NSPEC
                          3
         IS R
                    AT
NSPEC
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                    AT
                          4
NSPEC
         IS R
                          5
                    AT
NSPEC
         IS R
                    ΑT
                          6
NSPEC
                          7
         IS R
                    ΑT
NSPEC
         IS R
                    AT
                          8
NSPEC
                          9
         IS R
                    AT
NSPEC
         IS R
                    AT
                         10
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         IS C
                    AT
                         11
         IS C
NSPEC
                    AT
                         12
NSPEC
         IS C
                    AT
                         13
NSPEC
         IS C
                    AT
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NSPEC
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NSPEC
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                    AT
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NSPEC
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NSPEC
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NSPEC
         IS C
                    ΑT
                        28
```

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NSPEC IS C
               AT 29
NSPEC IS C
                 AT 30
NSPEC IS C
                 AT
                    31
NSPEC ' IS C
                 AT
                    32
               ΑT
                    33
NSPEC IS C
NSPEC IS C
               AT 34
NSPEC IS C
               AT 35
NSPEC IS C
                 AΤ
NSPEC IS C
                 AT
                    37
       IS C
NSPEC
                 AT 38
DEFAULT MLEVEL IS ATOM
MLEVEL IS CLASS AT 11 12 13 14 15 16 17 18 27 28 29 30 31 32 33 34 35
         36 37 38 39 40 41
DEFAULT ECLEVEL IS LIMITED
GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS 41
STEREO ATTRIBUTES: NONE
=> s 115
SAMPLE SEARCH INITIATED 01:52:41 FILE 'CASREACT'
SCREENING COMPLETE - 1 REACTIONS TO VERIFY FROM 1 DOCUMENTS
100.0% DONE
             1 VERIFIED
                              0 HIT RXNS
                                                              0 DOCS
SEARCH TIME: 00.00.01
FULL FILE PROJECTIONS: ONLINE **COMPLETE**
                              **COMPLETE**
                      BATCH
PROJECTED VERIFICATIONS:
                               1 TO
PROJECTED ANSWERS:
                               0 TO
L16
            0 SEA SSS SAM L15 ( 0 REACTIONS)
=> s 115 full
THE ESTIMATED SEARCH COST FOR FILE 'CASREACT' IS 102.30 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y) /N or END:y
FULL SEARCH INITIATED 01:52:46 FILE 'CASREACT'
SCREENING COMPLETE - 50 REACTIONS TO VERIFY FROM 12 DOCUMENTS
100.0% DONE
              50 VERIFIED 0 HIT RXNS
                                                              0 DOCS
SEARCH TIME: 00.00.01
L17
            0 SEA SSS FUL L15 ( 0 REACTIONS)
=>
```

h ebc gcgb